SEMESTER-IV SYLLABUS

PAPER – 1: MODERN SYNTHETIC METHODOLOGY IN ORGANIC CHEMISTRY

(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of modern synthetic methods,
CO 2: Understands various multicomponent reactions
CO 3: Develop the concept of click chemistry and Biorthogonal Chemistry
CO 4: Apply the knowledge and understanding the reactions of unactivated C-H bonds
CO 5: Acquire and understand various new methods in organic synthesis

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain and apply modern synthetic methods in preparing new molecules
LO 2: Analyze various multicomponent reactions
LO 3: Apply the new concept of click chemistry in organic synthesis and biological system
LO 4: Explain and apply the knowledge and understanding the reactions of unactivated C-H bonds,
LO 5: Solve and analyze new green chemistry methods in organic synthesis.
LO 6: Compare various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions

UNIT – I: Modern Synthetic Methods [12 Hours]

Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbeolefination. Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reaction.

UNIT-II: Multi component Reactions: [12 Hours]

Passerini reaction, Biginelli reaction, Hantzsch reaction and Mannich reaction. Metathesis: Grubb's 1st generation and 2nd generation catalyst, Olefin Cross coupling Metathesis (OCM), Ring Closing Metathesis (RCM), Ring Opening Metathesis (ROM) and applications.

UNIT-III: Click Chemistry: [12 Hours]

Introduction to click chemistry Copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC), Strain-promoted azide-alkyne cycloaddition (SPAAC), Strain-promoted alkyne-nitrone cycloaddition (SPANC)

Reactions of strained alkenes: Alkene and azide [3+2] cycloaddition, Alkene and tetrazine inverse-demand Diels-Alder, Biorthogonal Chemistry:

UNIT-IV: Reactions of unactivated carbon-hydrogen bonds: [12 Hours]

Unactivated carbon-hydrogen bonds: Definition, mechanism and synthetic applications- The
Hoffmann-Loeffler-Freytag reaction (HLF reaction)-cyclisation reactions of Nitrenes-the Barton reaction-Photolysis of organic hypohalites, hypochlorites, hypobromites and hypoiodites,

UNIT-V: newer methods in organic synthesis: [12 Hours]
Green Chemistry: Introduction, principles, atom economy and scope (illustrate with two examples) **Microwave induced reactions:** Principle conditions, advantages over conventional heating methods-applications **Ionic liquids:** Introduction and applications in organic synthesis (illustrate with two examples). **Nanomaterials:** Introduction, methods of preparation, applications in organic synthesis **Phase-transfer catalysis:** solid-solid, solid-liquid systems-mechanism of catalytic action, type of catalysts, application in few important reactions

Text Books:

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge
   University Press, Cambridge, 1988.
2. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
4. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley& Sons, 2003.
5. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley–VCH, New York, 2000.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
7. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
8. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis Elsevier Academic Press, 2005.
9. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
10. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
11. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Agarwal

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SEMESTER-IV SYLLABUS
PAPER II- ORGANIC SPECTROSCOPY AND PRINCIPLES OF INSTRUMENTATION
(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of ^{13}C NMR Spectroscopy
CO 2: Understand ^{13}C and Heteronuclear, 2D NMR and Instrumentation, learn FT NMR spectroscopy, 2D-NMR, COSY and HETCOR and their applications in molecular structure determination
CO 3: Develop interest in the areas, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
CO 4: Acquire interest in solving structures of organic molecules using 2D NMR, COSY, HETCOR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
CO 5: know the various chromatographic separation techniques. Principle and instrumentation of GC, HPLC and XRD

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain theory and values of ^{13}C NMR Spectroscopy
LO 2: Analyze and apply the concept of 2D NMR and Instrumentation, learn FT NMR spectroscopy, 2D-NMR, COSY and HETCOR in molecular structure determination
LO 3: Apply the concept of ORD and CD spectroscopy and structural determination of natural products by spectroscopy
LO 4: Interpret, Analyze and solve the structure of organic compounds using ^{13}C NMR, HNMR, 2D NMR, COSY and HETCOR.
LO 5: Explain various chromatographic separation techniques. Principle and instrumentation of GC, HPLC and XRD

UNIT-I: ^{13}C NMR spectroscopy [12 Hours]

Introduction, ^{13}C-chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and aromatic compounds. Types of ^{13}C NMR spectra: Proton-coupled, proton-decoupled and OFF-resonance decoupled (ORD) spectra, DEPT. ^{13}C-NMR solvents:

UNIT-II: NMR Instrumentation, 2D-NMR techniques [12 Hours]

NMR Instrumentation: Types of NMR Spectrometers-Continuous Wave (CW)-NMR, Fourier Transform (FT)-NMR, NMR solvents, sample preparation.

2D-NMR techniques: Principles of 2D NMR, Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY), Hetero COSY (^{1}H,^{13}C COSY, HMQC), long range ^{1}H,^{13}C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.

UNIT-III: Optical Rotatory Dispersion (ORD) and CD Spectroscopy: [12 Hours]

Optical rotation, circular birefringence, and circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Application of the rules to the study of absolute configuration and conformations of organic molecules.

UNIT-IV: Structure Determination of Natural Products by Spectral Methods [12 Hours]

Sructure elucidation - Spectroscopic techniques IR, UV, ^{1}H-NMR, ^{13}C-NMR, COSY, HETEROCOSY, and MS- natural products - Examples, flavones - Apigenin, flavanones-Hesperetin, isoflavones - Genistein, coumarins-7-hydroxycoumarin, alkaloids - morphine, quinine, terpenoids - (-)-Menthol, Steroids - stigmasterol, Glycosides - salicin (Alcoholic β-glucoside)

UNIT-V: Heteronuclear NMR spectroscopy and Principles of Instrumentation techniques [12 Hours]

Heteronuclear couplings: ^{13}C-^{1}H, ^{13}C-D, ^{13}C-^{19}F, ^{13}C-^{31}P. ^{1}H-D, ^{1}H-^{19}F, ^{1}H-^{31}P,
Instrumentation – Gas Chromatography - High Performance Liquid Chromatography - X – Ray Diffraction (XRD).

Text books:

1. Spectroscopy, fourth edition, D. L Pavia, G. M Lampman CENGAGE Learning, 2012
2. Spectroscopic Methods in Organic Chemistry. Fourth Edition D.M. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990. For all spectral methods except ORD and CD and ESR.
3. Organic Spectroscopy, Second Edition, W.Kemp, ELBS Macmillan, 1987 for ORD and CD and ESR.
4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010
   (For IV th unit)
5. Applications of absorption spectroscopy of Organic Compounds J.R.Dyer, Prentice Hall of India, New Delhi, 1984.
6. Spectrometric identification of Organic Compounds, Fourth Edition, R.M. Silverstein: G.C.Vassiellr and T.C. Merill, Johne Willey, Singapore, 1981.
7. For ORD and CD "Applications of Optical rotation and Circular Dichroism", G.C. Barret, in "Elucidation of Organic structures by Physical and Chemical Methods" Part I (Eds)
8. K.W. Bentley and G.W.Kirty John Wiley, 1972, Chapter VIII (only those aspects mentioned in the syllabus).

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SEMESTER-IV SYLLABUS
PAPER – III: DESIGNING ORGANIC SYNTHESIS AND SYNTHETIC APPLICATIONS OF ORGANO- BORANES AND SILANES
(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of principles of disconnection approach.
CO 2: Understands various synthetic strategies for one group disconnection.
CO 3: Understands various synthetic strategies for Two group disconnection.
CO 4: Develop knowledge on various organoboranes.
CO 5: Develop knowledge on various organosilanes.

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain and apply principles of disconnection approach.
LO 2: Apply in analyzing molecules using various synthetic strategies for one group disconnection.
LO 3: Analyze molecules using various synthetic strategies for one group disconnection.
LO 4: Apply different organoborane reagents in organic synthesis.
LO 5: Apply different organosilanes reagents in organic synthesis.
LO 6: Compare and apply the knowledge of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes.

UNIT-I: Disconnection Approach – Principles [12 Hours]

Introduction, Terminology: Retrosynthesis, Target Molecule (TM), synthon, synthetic equivalent, functional group interconversion (FGI). Linear and convergent synthesis. Criteria for selection of target. Order of events in retrosynthesis with reference to Salbutamol, Proparcaine and Dopamine. Chemoselectivity, Regioselectivity, reversal of polarity and cyclizations. Protecting groups- Principles of protection of alcohols, amine, carbonyl and carboxyl groups

UNIT-II: Synthetic Strategies - One group Disconnections [12 Hours]

Introduction to one group disconnections: C-C disconnection-alcohols and carbonyl compounds; C-X disconnections- alcohols and carbonyl compounds and sulphides two group C-C and C-X Disconnections.

UNIT-III: Synthetic Strategies - Two group Disconnections [12Hours]

Introduction to Two group C-C disconnections; Diels-Alder reaction, 1,5-difunctionalized compounds, Michael addition and Robinson annulation. Two group C-X disconnections; 1, 1-difunctionalised, 1, 2-difunctionalised and 1, 3-difunctionalised compounds. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid.

UNIT –IV: Organoboranes [12 Hours]

Hydroboration- Preparation of Organoboranes. Reagents – dicylohexyl borane, disiamyl borane, thexyl borane, 9-BBN and mono-, di-isopinocamphenyl borane. Functional group transformations of Organoboranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organoboranes-carbonylation, cyanoboration.

UNIT –V: Organosilanes [12 Hours]

Preparation and synthetic applications of trimethylsilyl chloride, dimethyl-t-butylsilylchloride, trimethylsilylcyanide, trimethylsilyliodide and trimethylsilyltriflate. Protection of functional groups - Trimethylsilylethers, Silylenolethers. Synthetic applications of α-silylcarbanions, β-silylcarbonium ions. Peterson's olefination.

Text Books:

1. Organic syntheses via boranes / Herbert C. Brown; with techniques by Gary W. Kramer,
2. Alan B. Levy, M. Mark Midland. New York: Wiley, 1975
3. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
4. Organic Synthesis: The disconnection approach, S. Warrant John Wiley & sons, New York, 1984.
5. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benzamine Inc. Menio Park, California, 1972.
6. Principle of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
7. Organic Synthesis: Special techniques. V.K. Ahulwalia and Renu Aggarwal.
8. Organic Synthesis by C Willis and M Willis
9. Problems on organic synthesis by Stuart Warren

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SEMESTER-IV SYLLABUS
PAPER IV-DRUG DESIGN AND DRUG CHEMISTRY
(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of basics of drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs,
CO 2: Understand the synthesis, mode of action, properties, uses and dosage of antineoplastic drugs,
CO 3: Understand the synthesis, mode of action, properties, uses and dosage of cardiovascular drugs
CO 4: Understand the synthesis, mode of action, properties, uses and dosage of oral hypoglycaemic drugs.
CO 5: Understand the synthesis, mode of action, properties, uses and dosage of local anti-infective and antiviral drugs

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain basics of drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs,
LO 2: Apply the mechanism of action, synthesis of antineoplastic drugs
LO 3: Apply the mechanism of action, synthesis of cardiovascular drugs
LO 4: Apply the mechanism of action, synthesis of hypoglycaemic drugs.
LO 5: Solve the structure and synthesis of local anti-infective and antiviral drugs
LO 6: Compare various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions

UNIT I: Introduction to Drugs [12 Hours]

General Classification, nomenclature, drug metabolism. Development of drugs: Procedure followed in drug design, concepts of lead compound lead modification, concept of prodrugs, Structure Activity Relationship (SAR)-factors affecting bio-activity-resonance, inductive effect, isosterism, bio-isosterism, spatial considerations, Quantitative Structure Activity Relationships (QSAR)-Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants,

UNIT II: Antineoplastic Agents: [12 Hours]

Introduction, classification-alkylating agents- mechanism and mode of action, nitrogen mustards-synthesis, properties, uses and dosage - Chlorambucil and melphalan. Antimetobolites- synthesis, properties, uses and dosage-pyrimidine analogues-5-flurouracil, purine analogues-6-mercaptopurine, folic acid analogues-Methotrexate. Antibiotics-structure, properties and dosage-Doxorubicin.

UNIT III: Cardiovascular Drugs: [12 Hours]

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

UNIT IV: Oral Hypoglycaemic Drugs: [12 Hours]

Introduction, Classification, Sulphonylureas- synthesis, mode of action, properties, uses and dosage- tolbutamide, glipizide. Biguanides- synthesis, mode of action, properties, uses and dosage-Metformin.α-glucosidage inhibitors- synthesis, mode of action, properties, uses and dosage- Miglitol. Dipeptidyl Peptidase-4 (DPP-4) inhibitors- synthesis, mode of action, properties, uses and dosage-saxagliptin and sitaglipti.

UNIT V: Local Anti-infective & Antiviral drugs [12 Hours]

Local Anti-infective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, ciprofloxacin, dapsone, amino salicylic acid, isoniazid, econazole and chloroquine.

Antiviral Drugs: Introduction, classification based on mechanism of action, Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NRTIs)-Synthesis, metabolism, properties and uses and dosage-Acyclovir, Zidovudine (Anti-HIV agent). Non-Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NNRTIs)-Synthesis, metabolism, properties and uses and dosage-Nevirapine, Efavirenz. Protease Inhibitors (PIs)- Synthesis, metabolism, properties and uses and dosage-Indinavir.

Text Books:

1. Text book of medicinal chemistry, Volume 1 & II, Third edition by V Alagarsamy, CBS-publishers
2. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
3. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
4. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.
5. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter.-9 and Ch-14), Ed. M. E. Wolff, John Wiley.
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
7. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
8. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

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DEPARTMENT OF ORGANIC CHEMISTRY

M.Sc. (Final) ORGANIC CHEMISTRY PRACTICALS
SEMESTER-IV
(Effective from 2023-2024 admitted batch)

Credits: 8		**Theory: 15 Hours**
Max Marks: 200	**External: 160**	**Internal: 40**

PRACTICAL SYLLABUS

Practical I

Analysis of six organic mixtures containing two components.

Practical II

Estimations and Isolation

a) Estimations
1) Estimation of Phenol
2) Estimation of Aniline
3) Estimation of Glucose
4) Estimation of Sucrose
5) Estimation of Aspirin
6) Estimation of Ibuprofen

b) Isolation
1) Isolation of Caffeine from tea leaves
2) Isolation of Piperine from pepper
3) Isolation of Lycopene from tamato

Text Books:

1. Vogel's Practical Organic Chemistry,
A.R. Tatchell, B.S. Furnis, A.J. Hannaford and P.W.G. Smith, 5th Edition, Pearson, New Delhi, 2017.

2. Vogel's Text book of Quantitative Inorganic Analysis,
J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th Edition, Pearson Education, New Delhi, 2008.

3. Chemistry of Natural Products: A Laboratory Handbook, N.R. Krishnaswamy, Universities Press, Hyderabad, 2013.

4. A Laboratory Manual of Organic Chemistry, R.K. Bansal, New Age International Publishers, New Delhi, 2008.

5. Practical Organic Chemistry, F.G. Mann & B.C. Saunders, Pearson, New Delhi, 2001.

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